Oscillateur harmonique à trois dimensions 2/2

1)

$$R_{n_r l}(r) = r^{-1} u_{n_r l}(r) = r^{-1} u_{\infty}(r) v_l(r)$$
$$= e^{-\frac{r^2}{2}} r^l \sum_{j=0}^{n_r} c_j r^{2j}$$

$$c_{j+1} = \frac{2l - 2n + 4j}{(4+4j)l + 6 + 10j + 4j^2} c_j = \frac{4j - 4n_r}{(4+4j)l + 6 + 10j + 4j^2} c_j$$

$$= \frac{-n_r + j}{(j+1)(l + \frac{3}{2} + j)}$$

$$\Rightarrow \underset{j=0}{c_1} = \frac{-n_r}{l + \frac{3}{2}} c_0 , \quad \underset{j=1}{c_2} = \frac{-n_r + 1}{2(l + \frac{5}{2})} c_1$$

$$\underset{j=2}{c_3} = \frac{-n_r + 2}{3(l + \frac{7}{2})} \dots$$

$\Rightarrow$ On reconnaît la fonction hypergéom. confluente dans le cas où elle vaut un polynôme de Laguerre généralisé

$$\Rightarrow R_{n_r l}(r) = e^{-\frac{r^2}{2}} r^l c_0 \left(1 + \frac{(-n_r)}{l + \frac{3}{2}} r^2 + \frac{(-n_r)(-n_r+1)}{(l+\frac{3}{2})(l+\frac{3}{2}+1) 2!} r^4 \right.$$

$$\left. + \frac{(-n_r)(-n_r+1)(-n_r+2)}{(l+\frac{3}{2})(l+\frac{3}{2}+1)(l+\frac{3}{2}+2) 3!} r^6 + \dots \right)$$

$$\Rightarrow R_{n_r l}(r) = e^{-\frac{r^2}{2}} r^l c_0 \, {}_1F_1\left(-n_r, l+\frac{3}{2}, r^2\right) = \tilde{c}_0 r^l e^{-\frac{r^2}{2}} L_{n_r}^{l+1/2}(r^2)$$

- n_r est le nombre de nœuds radiaux de la fonction $R_{n_r l}$ (c.à.d. le nombre de fois que la densité de prob. s'annule)

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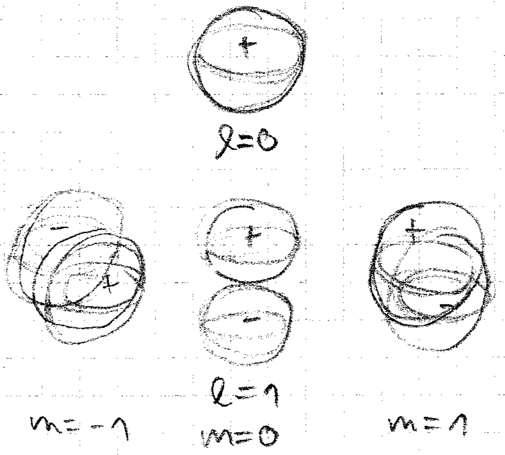
2) $\underline{n=0:}$

$$n = 2n_r + l = 0$$

$$\Rightarrow n_r = 0,\ l = 0$$

$$\Psi(\vec{r}) = e^{-\frac{r^2}{2}} c_0 Y_0^0(\Omega)$$

$Y_l^m(\Omega)$:



$$Y_l^m(\theta,\varphi) = \frac{1}{\sqrt{2\pi}} N_{lm} P_{lm}(\cos\theta) e^{im\varphi}$$

$$N_{lm} = \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}$$

$$P_{lm}(x) = \frac{(-1)^m}{2^l l!}(1-x^2)^{\frac{m}{2}}\frac{d^{l+m}}{dx^{l+m}}(x^2-1)^l$$

Polynome de Légendre

$l=0$: $$Y_0^0(\theta,\varphi) = \frac{1}{\sqrt{2\pi}}\sqrt{\frac{1}{2}} = \frac{1}{\sqrt{4\pi}}$$

$$\Rightarrow \Psi(\vec{r}) = \frac{e^{-\frac{r^2}{2}} c_0}{\sqrt{4\pi}}$$

Normalisation : $$\iiint d^3r\, |\Psi(\vec{r})|^2 = 1 = \underbrace{\int d\Omega\, |Y_0^0(\Omega)|^2}_{=1} \int_0^\infty dr\, r^2 |c_0|^2 e^{-r^2}$$

$$= |c_0|^2 \int_0^\infty dr\, r^2 e^{-r^2} = |c_0|^2 \int_0^\infty \frac{dt}{2\sqrt{t}}\, t\, e^{-t} = \frac{|c_0|^2}{2}\int_0^\infty dt\, t^{1/2} e^{-t}$$

$t = r^2$

$dt = 2r\,dr$

$$= \frac{|c_0|^2}{2}\Gamma(3/2) = \frac{|c_0|^2}{4}\Gamma(1/2) = \frac{|c_0|^2}{4}\sqrt{\pi}$$

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Répr. de pos. $|x\rangle$, rel. de ferm. $\int dx\, |x\rangle\langle x| = \mathbb{1}$

$$\Rightarrow |C_0| = \frac{2}{\pi^{1/4}} \qquad \Rightarrow |0_x\rangle = \int dx\, |x\rangle \underbrace{\langle x|0\rangle}_{\frac{1}{\pi^{1/4}} e^{-\frac{x^2}{2}}} = \int dx\, \frac{1}{\pi^{1/4}} e^{-\frac{x^2}{2}} |x\rangle$$

Rech: $\langle 0_x | 0_x \rangle = 1$ ..

$$\Rightarrow \boxed{\psi_{00}(\vec{r}) = \frac{1}{\pi^{3/4}} e^{-\frac{r^2}{2}} = \frac{e^{-\frac{x^2}{2}}}{\pi^{1/4}} \frac{e^{-\frac{y^2}{2}}}{\pi^{1/4}} \frac{e^{-\frac{z^2}{2}}}{\pi^{1/4}} \Rightarrow |0_x\rangle |0_y\rangle |0_z\rangle}$$

$\underline{n=1:}$ $n_r = 0$, $\ell = 1$

$$Y_1^m(\vartheta,\varphi) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3(1-m)!}{2(1+m)!}} \frac{(-1)^m}{2^1} (1-\cos^2\vartheta)^{\frac{m}{2}} \frac{d^{m+1}}{d\cos\vartheta^{m+1}} (\cos^2\vartheta - 1) e^{im\varphi}$$

$$R_{01}(r) = e^{-r^2/2}\, r\, C_0$$

$\underline{m=0:}$

$$Y_1^0(\vartheta,\varphi) = \frac{1}{\sqrt{2\pi}} \sqrt{\frac{3}{2}} \frac{d}{d\cos\vartheta} (\cos^2\vartheta - 1) = \sqrt{\frac{3}{4\pi}} \cos\vartheta$$

$$\psi_{n\ell m}(\vec{r}) = \psi_{010}(\vec{r}) = e^{-\frac{r^2}{2}}\, r\, C_0 \sqrt{\frac{3}{\pi}} \cos\vartheta$$

$$\int d^3r\, |\psi(\vec{r})|^2 = 1 = \underbrace{\int d\Omega\, Y_0^1(\vartheta,\varphi)}_{=1} \int_0^\infty dr\, r^4\, e^{-r^2} \cdot |C_0|^2 = \frac{|C_0|^2}{2} \Gamma\left(\frac{5}{2}\right) = 1$$

$$\Rightarrow C_0 = \frac{2\sqrt{2}}{\sqrt{3}\,\pi^{1/4}} \quad \Rightarrow \quad \boxed{\psi_{010}(\vec{r}) = \frac{\sqrt{2}}{\pi^{3/4}} e^{-r^2/2}\, r \cos\vartheta}$$

$$\boxed{\psi(\vec{r}) = \frac{2\sqrt{2}}{\sqrt{3}\,\pi^{1/4}} e^{-r^2/2}\, r\, Y_1^m(\Omega)}$$

$$= \frac{\sqrt{2}}{\pi^{3/4}} e^{-\frac{r^2}{2}} z$$

$$= \frac{e^{-\frac{x^2}{2}}}{\pi^{1/4}} \times \frac{e^{-y^2/2}}{\pi^{1/4}} \times \frac{2\sqrt{2}\, z}{\pi^{1/4}} e^{-\frac{z^2}{2}}$$

$$= |0_x\rangle |0_y\rangle |1_z\rangle$$

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<u>$m=-1$:</u>

$$Y_1^{-1}(\vartheta,\varphi) = -\frac{1}{\sqrt{2\pi}}\sqrt{3}\,\frac{1}{\sqrt{1-\cos^2\vartheta}}\left(\cos^2\vartheta-1\right)e^{-i\varphi} = -\sqrt{\frac{3}{8\pi}}\,\frac{(\cos^2\vartheta-1)}{\sqrt{1-\cos^2\vartheta}}\,e^{-i\varphi}$$

$$\Rightarrow \Psi_{01-1}(\vec{r}) = -\frac{2\sqrt{2}\,\cancel{\sqrt{8}}}{\cancel{\sqrt{3}}\,\pi^{1/4}}\,\frac{\cancel{\sqrt{3}}}{\cancel{\sqrt{8}}\,\pi}\,e^{-r^2/2}\,r\,\frac{(\cos^2-1)}{\sqrt{1-\cos^2\vartheta}}\,e^{-i\varphi}$$

$$= -\frac{1}{\pi^{3/4}}\,e^{-r^2/2}\,r\,\underbrace{\frac{\overbrace{(\cos^2-1)}^{-\sin^2\vartheta}}{\sqrt{1-\cos^2\vartheta}}}_{\sin\vartheta}\,e^{-i\varphi} =$$

$$\boxed{\Psi_{01-1}(\vec{r}) = +\frac{1}{\pi^{3/4}}\,e^{-\frac{r^2}{2}}\,r\,\sin\vartheta\,e^{-i\varphi}}$$

$$= +\frac{1}{\pi^{3/4}}\,e^{-\frac{r^2}{2}}(-x+iy) \Rightarrow \frac{1}{\sqrt{2}}\left(|1_x\rangle|0_y\rangle|0_z\rangle - i|0_x\rangle|1_y\rangle|0_z\rangle\right)$$

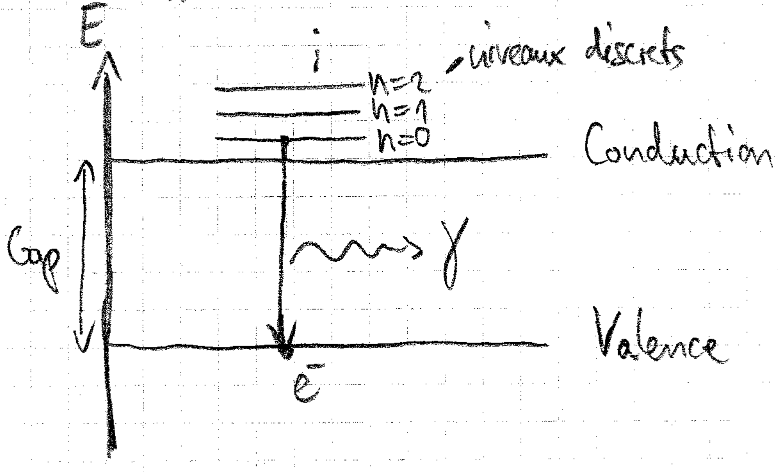
<u>$m=+1$:</u>

$$\boxed{Y_1^1(\vartheta,\varphi) = -\frac{1}{\pi^{3/4}}\,e^{-r^2/2}\,r\,\sin\vartheta\,e^{+i\varphi}} = -\frac{\cancel{1}\sqrt{2}}{\pi^{3/4}}\,e^{-\frac{r^2}{2}}(x+iy)$$

$$\Rightarrow -\frac{1}{\sqrt{2}}\left(|1_x\rangle|0_y\rangle|0_z\rangle + i|0_x\rangle|1_y\rangle|0_z\rangle\right)$$

3)

Application numérique :



Energie fondamentale dans la bande de conduction :

$$E_0 = \frac{3}{2}\hbar\omega$$

$\Rightarrow$ Energie minimale d'un photon émis par un e^- passant de l'état de conduction le plus bas à l'état de valence le plus élevé :

$$E_{min} = E_{gap} + E_0 = 1{,}42\,eV + 6\,meV = 1{,}426\,eV$$

Energie du photon : $E_\gamma = \hbar\omega = h\nu \Rightarrow \nu \approx 2{,}17 \cdot 10^{15}\,Hz$

$\Rightarrow \lambda \approx 138\,nm$

(ultraviolet proche)